# A Bound and Estimate for the Maximum Compression of Single Shocks

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Abstract

We derive that the compression for any single shock has an upper bound of 7. This is in the case of shocking from any initial state except gaseous densities with temperatures such that a significant fraction of the electrons are bound. For shocks in condensed material initially near ambient, we present a simple analytic estimate for the maximum compression as a function of $\rho_o$ (initial density), $A$ (atomic weight), $Z$ (atomic number), and $\Delta E$ (the sum of cohesion, dissociation, and total ionization energies).

## Introduction

For any material that is compressed by a shock wave, one might suppose that increasing the pressure of the shock wave to arbitrarily high values will produce an arbitrarily large compression. This is not true and in particular one can show that for infinitely strong shock waves in any substance there is a compression of exactly fourfold from the initial density in front of the shock to the final density behind the shock. Thus in defiance of the high pressure, the compression is limited by the high temperatures produced by shocks. For condensed materials shocked from near ambient the maximum possible compression attainable by a single shock is greater than four and occurs at some finite pressure, the particular values depending on the specific material and on the initial density and temperature. This overshot of the fourfold limit is caused by the “softening” of the material when energy is drained into internal degrees of freedom such as in ionization.

In this note we derive from general arguments an upper bound on the maximum compression attainable by a single shock in any material from any initial state except those with gaseous densities and a significant number of bound electrons. We also obtain an estimate of the maximum compression in the case of condensed materials shocked from near ambient.

## An Upper Bound

A Hugoniot is a curve in thermodynamic parameter space that is the collection of final states behind a shock as the strength of a shock is varied for fixed initial state. Hugoniots, along with isotherms, isobars, and isentropes, for example, are curves specified on the equation of state surface by constraints such as requiring that the temperature, pressure, or entropy is constant. It is just that the constraint for the Hugoniot is not as simple as keeping a standard thermodynamic variable fixed. For weaker shocks with little entropy production the Hugoniot is approximately an isentrope. For shocks with significant entropy production the Hugoniot in pressure-density space is stiffer than an isentrope. The principal Hugoniot is that one with ambient as the initial state [1].

Any Hugoniot is determined from the hydrodynamic equation of state $P(\rho,E)$ and the energy jump constraint,

$$E - E_o = \frac{1}{2}\left(P + P_o\right)\left(1/\rho_o - 1/\rho\right) \quad . \tag{1}$$

Here $P$ is pressure, $\rho$ is density, and $E$ is the internal energy per gram. $P_o$, $\rho_o$, and $E_o$ represent the same but are for the initial state of the Hugoniot. We define the compression as $\eta = \rho/\rho_o$ and rewrite Eq. (1) as

$$\eta = 4 + \left[2\rho\left(E - E_o\right) - 3\left(P + P_o\right)\right]/\left(P + P_o\right) \quad . \tag{2}$$

We now assume that the virial theorem is exact for the equation of state [2]; i.e., if $E = K + U$, where $K$ is the average kinetic energy per gram and $U$ is the average potential energy per gram, then $P/\rho = 2K/3 + U/3$. (We are considering here the case of physical interest, namely, the charge neutral, quantum Coulomb system.) Substituting into Eq. (2), we get

$$\eta = \eta_b - 3P_o\left(1 + \eta\right)/\left(P + P_o\right) \le \eta_b \quad , \tag{3}$$

where $\eta_b = 4 + \rho(U - U_o)/(P + P_o)$. If $U \le U_o$, then $\eta \le \eta_b \le 4$. If $U \ge U_o$, then we rewrite Eq. (3) as

$$\eta \le \eta_b = 4 + 3/\left[1 + 2K_s/U_s + 3P_o\left(1/\rho + 1/\rho_o\right)/U_s\right] \ , \tag{4}$$

where $K_s = K - K_o$ and $U_s = U - U_o$.

For classical systems, $K_s \ge 0$ because the average kinetic energy is linear in temperature $T$. This is not the case in general for a quantum, charge neutral, bare Coulomb system. For low densities where atomic states are a good approximation for the electrons, the electrons ionize from localized high kinetic energy states to low kinetic energy extended free states. Thus the average kinetic energy drops as the temperature rises as long as there is a significant fraction of electrons remaining to be ionized. This is nothing more than the uncertainty principle with the electrons going from a small to a big box. The just discussed situation is not the case for densities higher than gaseous. There the electrons do not have an extreme change in localization in going from low to high temperatures. Thus for quantum systems, it is very reasonable that $K_s \geq 0$ when $U_s \geq 0$ if $\eta \geq 7 - \varepsilon$ ($\varepsilon > 0$) for a material shocked from densities greater than gaseous. (Models support this position.) Then from Eq. (4), $\eta \leq \eta_b \leq 7$. Thus we conclude that the compression along a single-shock Hugoniot for any material cannot exceed 7 for a broad class of initial shock states.

## An Estimate for the Principal Hugoniot

We now look to the principal Hugoniot, where $P_o = 0$. We assume that we are shocking from $T = 0$. (The difference between zero and room temperature is small when we are looking for estimates of the maximum compression.) From Eqs. (3) and (4), we find that

$$\eta = 4 + 3/(1 + 2K_s/U_s) \ . \tag{5}$$

It is convenient to define $Y = U_s/(2\Delta E)$ where, for the principal Hugoniot, $\Delta E = -E_o$ and is the sum of cohesive, dissociation, and total ionization energies. Then

$$\eta = (7Y + 4K_s/\Delta E)/(Y + K_s/\Delta E) \ . \tag{6}$$

From the exact high-temperature series for the equation of state of any elemental material [3], we obtain $Y$ as an exact series in $1/K_s$. (We are thinking of $K_s$ as the independent variable.) All that we need is

$$Y = 1 + a\alpha^{1/2} + \qquad , \tag{7a}$$

with

$$a = -e^3 (1+Z)^2 (L/A)^2 / \Delta E \tag{7b}$$

and

$$\alpha = 3\pi Z^3 \rho_o /(2K_s) \quad . \tag{7c}$$

In these equations, $L$ is Avogadro's number, and $e$ is the electron charge. The $a\alpha^{1/2}$ originates from the Debye-Hückel term in the high-$T$ expansion.

We substitute Eqs. (7a)-(7c) into Eq. (6) and solve for the maximum compression, $\eta_m$. The result is

$$\eta_m = 4(1+7C)/(1+4C) \quad , \tag{8a}$$

with

$$C = 2(\Delta E / Z)^3 A^4 /[81 e^6 \pi (1+Z)^4 L^4 \rho_o] \quad . \tag{8b}$$

This is our estimate for the maximum compression along the principal Hugoniot.

Equation (8b) can be simplified further if one neglects cohesive and dissociation energies. We fit to the total ionization energies of C. E. Moore (through Ca) [4] to estimate that $\Delta E \approx 13.6\ Z^{2.4}$ eV per atom. Thus

$$C \approx 0.011 A Z^{4.2} /[\rho_o (1+Z)^4] \quad . \tag{8c}$$

## Conclusions

The estimates of Eqs. (8a)-(8c) and an upper bound of 7 are our results. The only existing data that is a strong test of our $\eta_m$ expression is for Al [5]. In that case $\eta_m \approx 5$, and that value agrees well with Eqs. (8). One has available more terms in the expansion Eq. (7a). We have extensively studied these terms and found that they do not influence our estimates at all. We have also extensively worked with the series Eq. (7a) using Padé approximants. Again there was no significant influence. We feel Eqs. (8a)-(8c) are a quite good approximation of $\eta_m$.

In a previous discussion of the high pressure Hugoniot [6], we presented the relations $s = 1 + \gamma/2$ and $\eta_m = 1 + 2/\gamma$, where $s$ is the derivative of the shock velocity with respect to the particle velocity and $\gamma = 1/\rho \, \partial P/\partial E|_\rho$ is the Grüneisen parameter. These relations are exact at any point on the Hugoniot where the density derivative of the pressure is infinite. The first is also approximately true for any given material over a very large region of the Hugoniot, including particle velocities from about 10 to 100 km/s. In such a region it is universal that $s \approx 1.2$ and thus $\gamma \approx 0.4$. It is above this very linear region that the Hugoniot becomes steeper and in pressure-density space attains maximum compression. There $s$ will be a little larger than its value in the linear region. (We should clarify that there are two linear regions in the shock velocity-particle velocity Hugoniot. One is from 0 to about 3 km/s for the particle velocity and the other, which is the one of interest, is from about 10 to 100 or more km/s.) From our approximation of the maximum compression and the above two relations, we can obtain estimates of $s$ and $\gamma$ at the maximum compression point. The ultimate limiting values for shocks of infinite strength are $\eta = 4$, $s = 4/3$, and $\gamma = 2/3$.

## References


[1] For more discussion see, for example, J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954), p. 398.

[2] We especially prefer the physics derivation of J. Yvon, Acad. Sci. (Paris) 227, 763(1948).

[3] See, for example, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, Inc., New York, 1971) p. 267.

[4] C. E. Moore, "Ionization Potentials and Ionization Limits Derived from the Analysis of Optical Spectra," Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 35 (1970).

[5] A. S. Vladimirov, N. P. Voloshin, V. N. Nogin, A. V. Petrovtsev, and V. A. Simonenko, Sov. Phys. JETP Lett. 39, 85 (1984).

[6] J. D. Johnson, *Shock Compression of Condensed Materials–1997*, (AIP, Woodbury, New York, 1998), pp. 27-30 and *General Features of Hugoniots–II,* Los Alamos report LA-13217-MS, January 1997 (unpublished).